LA-UR-13-23152

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Title:	Fission Matrix Capability for MCNP, Part I - Theory
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Intended for:	M & C 2013 - ANS Mathematics & Computations Division Topical Meeting, 2013-05-05/2013-05-09 (Sun Valley, Idaho, United States) MCNP documentation Report Web
Issued:	2013-05-01

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Fission Matrix Capability for MCNP, Part I - Theory

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Abstract

Fission Matrix Capability for MCNP, Part I – Theory

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The theory underlying the fission matrix method is derived using a rigorous Green's function approach. The method is then used to investigate fundamental properties of the transport equation for a continuous-energy physics treatment. We provide evidence that an infinite set of discrete, real eigenvalues and eigenfunctions exist for the continuous-energy problem, and that the eigenvalue spectrum converges smoothly as the spatial mesh for the fission matrix is refined. We also derive equations for the adjoint solution. We show that if the mesh is sufficiently refined so that both forward and adjoint solutions are valid, then the adjoint fission matrix is identical to the transpose of the forward matrix. While the energy-dependent transport equation is strictly biorthogonal, we provide surprising results that the forward modes are very nearly self-adjoint for a variety of continuous-energy problems. A companion paper (Part II – Applications) describes the initial experience and results from implementing this fission matrix capability into the MCNP Monte Carlo code.

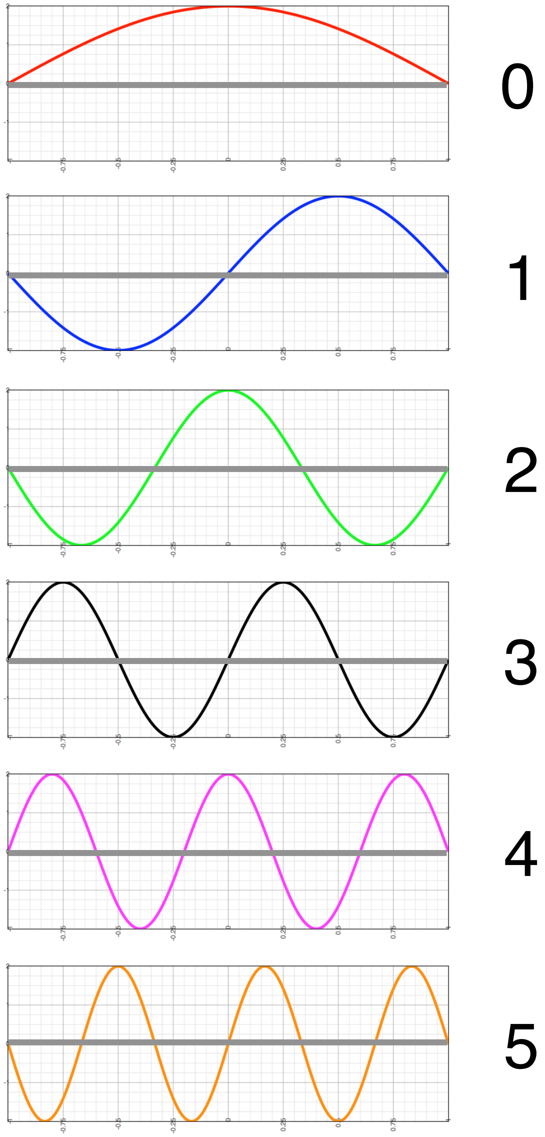
- **Introduction**
  - Higher eigenmodes
  - Green's functions & transport
  - Motivation
- **Theoretical Basis of the Fission Matrix**
  - Integral equation for the neutron source
  - Integral equation for the adjoint source
  - Comments of forward vs adjoint
- **Forward & Adjoint Fission Matrix Equations**
  - Forward fission matrix equations
  - Adjoint fission matrix equations
  - Relationship between forward & adjoint
- **Fission Matrix Eigenmodes & Eigenvalue Spectrum**
  - Higher mode analysis
  - Spectrum convergence with mesh refinement
  - Real vs Complex eigenvalues
  - Near-orthogonality of eigenfunctions
- **Conclusions & Future Work**

Carney, Brown, Kiedrowski, Martin, “Fission Matrix Capability for MCNP Monte Carlo”, TANS 107, San Diego, 2012

Carney, Brown, Kiedrowski, Martin, “Fission Matrix Capability for MCNP, Part II - Applications”, M&C-2013, 2013

Introduction

Introduction - Higher Eigenmodes



etc.

Vibrating strings:

- Higher modes add "tone", but die away quickly
- **Fundamental mode persists**
- Feedback, instability, nonlinear effects, …, may excite higher modes

Introduction - Green's Functions & Transport Theory

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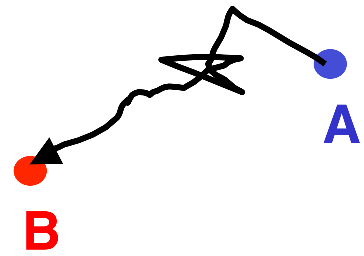


$$S_B = S_A \cdot F(A \rightarrow B)$$

- **F(A→B)**
  - **Green's function, "here-to-there" function**
  - **Probability that source at point A produces source at point B**

- **Transport theory - Peierl's equation for multiplying system**

$$S(\vec{r}) = \frac{1}{k_{eff}} \cdot \int_{\text{all } \vec{r}'} d\vec{r}' \cdot S(\vec{r}') \cdot F(\vec{r}' \rightarrow \vec{r})$$

  - **Discretize space into blocks, or mesh regions**
  - **Compute F(r'→r) with Monte Carlo**
  - **Solve matrix eigenvalue problem for sources:**

$$\vec{S} = \frac{1}{k_{eff}} \cdot \bar{F} \cdot \vec{S}$$

  - **Can also solve for higher modes**

Introduction – Who Cares?

- **Knowledge of fundamental & all higher modes**
  - "Crown Jewels" of analysis – explains everything

- **Reactor theory & mathematical foundations**
  - Existence of higher modes
  - Eigenvalue spectrum – discrete ? real ?
  - Forward & adjoint modes
  - Assessment of spatial refinement

- **Fundamental reactor physics analysis**
  - Higher modes for stabiility analysis of Xenon & void oscillations
  - Slow-transient analysis
  - Startup, probability of initiation

- **Source convergence testing & acceleration**
  - May provide robust, reliable, automated convergence test
  - Acceleration of source convergence

Theoretical Basis of the Fission Matrix

Integral Equation for the Neutron Source (1)

- **Transport equation, k-eigenvalue form**

$$M \cdot \Psi(\vec{r},E,\hat{\Omega}) = \tfrac{1}{K} \cdot \frac{\chi(E)}{4\pi} \cdot S(\vec{r})$$

M = net loss operator

$$M \cdot \Psi(\vec{r},E,\hat{\Omega}) = \hat{\Omega} \cdot \nabla\Psi(\vec{r},E,\hat{\Omega}) + \Sigma_T(\vec{r},E)\Psi(\vec{r},E,\hat{\Omega}) \\ - \iint dE'\, d\hat{\Omega}' \;\Sigma_S(\vec{r},E' \to E,\hat{\Omega}' \to \hat{\Omega})\; \Psi(\vec{r},E',\hat{\Omega}')$$

S(r) = fission neutron source

$$S(\vec{r}) = \iint dE'\, d\hat{\Omega}' \;\nu\Sigma_F(\vec{r},E')\; \Psi(\vec{r},E',\hat{\Omega}')$$

χ(E) = emission spectrum,
following analysis is same if replaced by

$$\chi(E,\vec{r}) = \frac{\iint dE'\, d\hat{\Omega}' \;\chi(E' \to E)\; \nu\Sigma_F(\vec{r},E')\; \Psi(\vec{r},E',\hat{\Omega}')}{\iint dE'\, d\hat{\Omega}' \;\nu\Sigma_F(\vec{r},E')\; \Psi(\vec{r},E',\hat{\Omega}')}$$

Integral Equation for the Neutron Source (2)

- **Define Green's function & integral transport equation**

$$M \cdot G(\vec{r}_0, E_0, \hat{\Omega}_0 \rightarrow \vec{r}, E, \hat{\Omega}) = \delta(\vec{r} - \vec{r}_0) \cdot \delta(E - E_0) \cdot \delta(\hat{\Omega} - \hat{\Omega}_0),$$

$$\Psi(\vec{r}, E, \hat{\Omega}) = \tfrac{1}{K} \cdot \iiint d\vec{r}_0\, dE_0\, d\hat{\Omega}_0\, \frac{\chi(E_0)}{4\pi} \cdot S(\vec{r}_0) \cdot G(\vec{r}_0, E_0, \hat{\Omega}_0 \rightarrow \vec{r}, E, \hat{\Omega})$$

- **Multiply by $\nu\Sigma_F(r,E)$, integrate over E, Ω**
- **Define energy-angle averaged Source & Green's function**

$$H(\vec{r}_0 \rightarrow \vec{r}) = \int \iiint dE\, d\hat{\Omega}\; dE_0\, d\hat{\Omega}_0 \cdot \nu\Sigma_F(\vec{r}, E) \cdot \frac{\chi(E_0)}{4\pi} \cdot G(\vec{r}_0, E_0, \hat{\Omega}_0 \rightarrow \vec{r}, E, \hat{\Omega})$$

$$S(\vec{r}) = \iint dE'\, d\hat{\Omega}' \cdot \nu\Sigma_F(\vec{r}', E') \cdot \Psi(\vec{r}', E', \hat{\Omega}')$$

$$S(\vec{r}) = \frac{1}{K} \int d\vec{r}_0 \cdot S(\vec{r}_0) \cdot H(\vec{r}_0 \rightarrow \vec{r})$$

$H(r_0 \rightarrow r)$ can be tallied directly in MC simulation

Integral Equation for the Adjoint Neutron Source (1)

- **Adjoint transport equation, k-eigenvalue form**

$$M^{\dagger} \cdot \Psi^{\dagger}(\vec{r},E,\hat{\Omega}) = \tfrac{1}{K} \cdot \frac{\nu\Sigma_F(\vec{r},E)}{4\pi} \cdot S^{\dagger}(\vec{r})$$

$M^{\dagger}$ = adjoint to operator M

$$\begin{aligned} M^{\dagger} \cdot \Psi^{\dagger}(\vec{r},E,\hat{\Omega}) = \; & -\hat{\Omega} \cdot \nabla\Psi^{\dagger}(\vec{r},E,\hat{\Omega}) + \Sigma_T(\vec{r},E)\Psi^{\dagger}(\vec{r},E,\hat{\Omega}) \\ & - \iint dE'\, d\hat{\Omega}' \cdot \Sigma_S(\vec{r},E \to E',\hat{\Omega} \to \hat{\Omega}') \cdot \Psi^{\dagger}(\vec{r},E',\hat{\Omega}') \end{aligned}$$

$S^{\dagger}$ (r) = adjoint fission neutron source

$$S^{\dagger}(\vec{r}) = \iint dE'\, d\hat{\Omega}' \cdot \frac{\chi(E')}{4\pi} \cdot \Psi^{\dagger}(\vec{r},E',\hat{\Omega}')$$

Bell & Glasstone & others have shown that forward & adjoint K eigenvalues are the same, $K^{\dagger} = K$, so will just use K in the following analysis.

Integral Equation for the Adjoint Neutron Source (2)

- **Adjoint Green's function & integral transport equation**

$$M^\dagger \cdot G^\dagger(\vec{r}_0, E_0, \hat{\Omega}_0 \to \vec{r}, E, \hat{\Omega}) = \delta(\vec{r} - \vec{r}_0) \cdot \delta(E - E_0) \cdot \delta(\hat{\Omega} - \hat{\Omega}_0)$$

$$\Psi^\dagger(\vec{r}, E, \hat{\Omega}) = \tfrac{1}{K} \cdot \iiint d\vec{r}_0\, dE_0\, d\hat{\Omega}_0 \cdot \nu\Sigma_F(\vec{r}_0, E_0) \cdot S^\dagger(\vec{r}_0) \cdot G^\dagger(\vec{r}_0, E_0, \hat{\Omega}_0 \to \vec{r}, E, \hat{\Omega})$$

- **Multiply by $\chi(E)$, integrate over E, Ω**
- **Define energy-angle averaged adjoint Source & Green's function**

$$H^\dagger(\vec{r}_0 \to \vec{r}) = \int \iiint dE\, d\hat{\Omega}\, dE_0\, d\hat{\Omega}_0 \cdot \frac{\chi(E)}{4\pi} \cdot \nu\Sigma_F(\vec{r}_0, E_0) \cdot G^\dagger(\vec{r}_0, E_0, \hat{\Omega}_0 \to \vec{r}, E, \hat{\Omega})$$

$$S^\dagger(\vec{r}) = \iint dE'\, d\hat{\Omega}' \cdot \frac{\chi(E')}{4\pi} \cdot \Psi^\dagger(\vec{r}', E', \hat{\Omega}')$$

$$S^\dagger(\vec{r}) = \frac{1}{K} \int d\vec{r}_0 \cdot S^\dagger(\vec{r}_0) \cdot H^\dagger(\vec{r}_0 \to \vec{r})$$

$H^\dagger$ ($r_0 \to r$) can be tallied directly in MC simulation

Forward & Adjoint Integral Equations for Source

- **Reciprocity for direct & adjoint Green's function**

$$G^{\dagger}(\vec{r}_0, E_0, \hat{\Omega}_0 \rightarrow \vec{r}, E, \hat{\Omega}) = G(\vec{r}, E, \hat{\Omega} \rightarrow \vec{r}_0, E_0, \hat{\Omega}_0)$$

Because of irreversible energy dependence, neither G nor $G^{\dagger}$ is symmetric in initial and final arguments. Same is true for H and $H^{\dagger}$

$$H^{\dagger}(\vec{r}_0 \rightarrow \vec{r}) = H(\vec{r} \rightarrow \vec{r}_0)$$

$$H(\vec{r}_0 \rightarrow \vec{r}) \neq H(\vec{r} \rightarrow \vec{r}_0),$$
$$H^{\dagger}(\vec{r}_0 \rightarrow \vec{r}) \neq H^{\dagger}(\vec{r} \rightarrow \vec{r}_0)$$

- **Using reciprocity, comparing H and $H^{\dagger}$ gives**

$$S(\vec{r}) = \frac{1}{K} \int d\vec{r}_0 \cdot S(\vec{r}_0) \cdot H(\vec{r}_0 \rightarrow \vec{r})$$

$$S^{\dagger}(\vec{r}) = \frac{1}{K} \int d\vec{r}_0 \cdot S^{\dagger}(\vec{r}_0) \cdot H(\vec{r} \rightarrow \vec{r}_0)$$

- **S and $S^{\dagger}$ are bi-orthogonal**

$$(K_p - K_q) \cdot \int d\vec{r} \cdot S_p(\vec{r}) \cdot S_q^{\dagger}(\vec{r}) = 0$$

K-eigenvalue Form of Transport Equation

$$M \cdot \Psi(\vec{r}, E, \hat{\Omega}) = \tfrac{1}{K} \cdot \frac{\chi(E)}{4\pi} \cdot S(\vec{r})$$

- **Structure & properties**
  - **60+ years ago:**
    A single, non-negative, real, fundamental eigenfunction & eigenvalue exist
  - **50+ years ago:**
    For 1-speed or 1-group: A complete set of self-adjoint, real eigenfunctions & discrete eigenvalues exists
  - **Energy-dependent transport equation is bi-orthognal, forward & adjoint modes are orthogonal**
  - **Nothing else proven, always assumed that higher-mode solutions exist**

- **In the present work based on the Fission Matrix:**
  - **We provide evidence that higher modes exist, are real, have discrete eigenvalues, and are very nearly self-adjoint (for reactor-like problems)**
  - **Approach is similar to Birkhoff's original proof for fundamental mode**
  - **This has never been done before using continuous-energy Monte Carlo**

Forward & Adjoint Fission Matrix Equations

Forward Fission Matrix Equations (1)

- **Segment the physical problem into N disjoint spatial regions**
  - Initial regions (r_0) for fission neutron source emission
  - Final regions (r) for production of a **next-generation** fission neutron

- **Integrate the forward integral fission source equation over r_0 & r**
  - Initial: $r_0 \in V_J$, Final: $r \in V_I$

$$S_I = \frac{1}{K} \cdot \sum_{J=1}^{N} F_{I,J} \cdot S_J$$

$$F_{I,J} = \int_{\vec{r} \in V_I} d\vec{r} \int_{\vec{r}_0 \in V_J} d\vec{r}_0 \frac{S(\vec{r}_0)}{S_J} \cdot H(\vec{r}_0 \to \vec{r}) \qquad S_J = \int_{\vec{r}' \in V_J} S(\vec{r}') d\vec{r}'$$

Exact equations for integral source S_I

N = # spatial regions, F = N x N matrix, <u>non</u>symmetric

Forward Fission Matrix Equations (2)

- $F_{I,J}$ = **next-generation fission neutrons produced in region I, for each average fission neutron starting in region J (J→I)**

- **In the equation for F,**
  - $S(r_0)/S_J$ is a local weighting function within region J
  - **As $V_J \rightarrow 0$:**
    - $S(r_0) \rightarrow S_J / V_J$
    - **Discretization errors → 0**
    - **Can accumulate tallies of $F_{I,J}$ even if not converged**

- **$F_{I,J}$ tallies:**
  - Previous F-matrix work: tally during neutron random walks
  - **Present F-matrix work: tally only point-to-point, using fission-bank in master proc (~free)**
    - Eliminates excessive communications for parallel
    - Provides more consistency, $F_{I,J}$ nonzero only in elements with actual sites
    - Analog-like treatment, better for preserving overall balance

Adjoint Fission Matrix Equations

- **Segment the physical problem into N disjoint spatial regions**
  - Initial regions: $r_0 \in V_J$, Final regions: $r \in V_I$

- **Integrate the adjoint integral fission source equation over r_0 & r**

$$S_I^\dagger = \frac{1}{K} \cdot \sum_{J=1}^{N} F_{I,J}^\dagger \cdot S_J^\dagger$$

$$F_{I,J}^\dagger = \int_{\vec{r} \in V_I} d\vec{r} \int_{\vec{r}_0 \in V_J} d\vec{r}_0 \frac{S^\dagger(\vec{r}_0)}{S_J^\dagger} \cdot H(\vec{r} \to \vec{r}_0) \qquad S_J^\dagger = \int_{\vec{r}' \in V_J} S^\dagger(\vec{r}')\, d\vec{r}'$$

Exact equations for adjoint integral source $S^\dagger_I$

Relationship Between Forward & Adjoint Fission Matrix

- **Compare $F_{I,J}$ & $F^{\dagger}_{J,I}$, interchange integration order for $F^{\dagger}_{J,I}$**

$$F_{I,J} = \int_{\vec{r} \in V_I} d\vec{r} \int_{\vec{r}_0 \in V_J} d\vec{r}_0 \cdot \frac{S(\vec{r}_0)}{S_J} \cdot H(\vec{r}_0 \to \vec{r})$$

$$F^{\dagger}_{J,I} = \int_{\vec{r}_0 \in V_J} d\vec{r}_0 \int_{\vec{r} \in V_I} d\vec{r} \cdot \frac{S^{\dagger}(\vec{r})}{S^{\dagger}_I} \cdot H(\vec{r}_0 \to \vec{r})$$

Same form, but different spatial weighting functions

- **If the spatial discretization is fine enough that**

$$\frac{S(\vec{r}_0)}{S_J / V_J} \approx 1 \quad \text{for } \vec{r}_0 \in V_J \qquad \text{and} \qquad \frac{S^{\dagger}(\vec{r})}{S_I / V_I} \approx 1 \quad \text{for } \vec{r} \in V_I$$

then

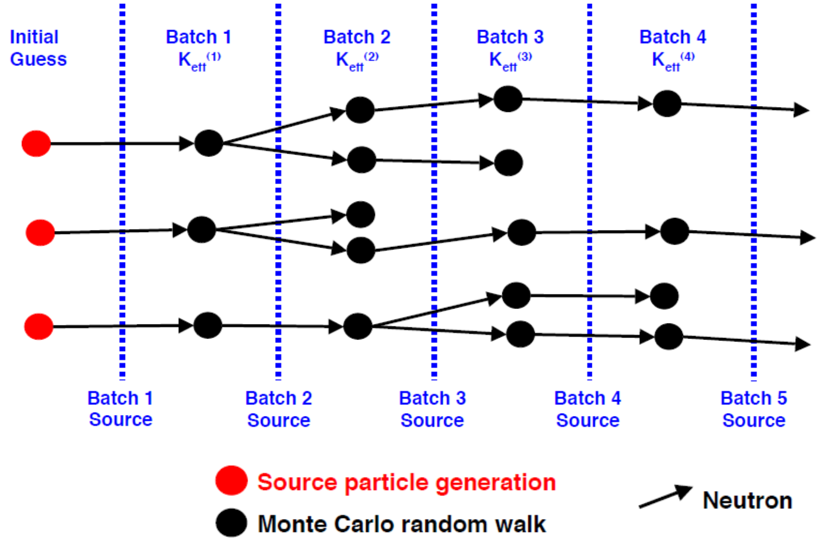
$$\bar{\bar{F}}^{\dagger} = \bar{\bar{F}}^{T}$$

For fine spatial mesh, $F^{\dagger}$ = transpose of F

Monte Carlo Estimation of Fission Matrix

Monte Carlo K-effective Calculation

1. Start with fission source & k-eff guess
2. Repeat until converged:
   - Simulate neutrons in cycle
   - Save fission sites for next cycle
   - Calculate k-eff, renormalize source
3. Continue iterating & tally results



For Fission Matrix calculation

During standard k-eff calculation, at the end of each cycle:

- Estimate $F_{I,J}$ tallies from start & end points in fission bank (~ free)
- Accumulate $F_{I,J}$ tallies, over all cycles (even inactive cycles)
- Normalize $F_{I,J}$ accumulators, divide by total sources in J regions
- Find eigenvalues/vectors of F matrix (power iteration, with deflation)

Fission Matrix Eigenmodes

&

Eigenvalue Spectrum

- **Run Monte Carlo, get fission matrix, then solve for eigenvalues & eigenfunctions**
  - Matlab, if full-storage **F** matrix can fit in memory
  - Power iteration with deflation, if sparse-format **F** matrix required

$$\vec{S}_n = \frac{1}{K_n} \cdot \bar{F} \cdot \vec{S}_n \qquad k_0 > |k_1| > |k_1| \; ... > |k_N|$$

$$\vec{S}_n^\dagger = \frac{1}{K_n} \cdot \bar{F}^T \cdot \vec{S}_n^\dagger \qquad n = 0,1,...N$$

$$(k_p - k_q) \cdot (\vec{S}_p \cdot \vec{S}_q^\dagger) = 0$$

  - **F** is <u>non</u>symmetric
  - $\mathbf{S_n}$ is a **right** eigenvector of **F**, $\mathbf{S^\dagger{}_n}$ is a **left** eigenvector of **F**
  - $\mathbf{S_n}$ and $\mathbf{S^\dagger{}_m}$ are biorthogonal

Whole-core 2D PWR Model

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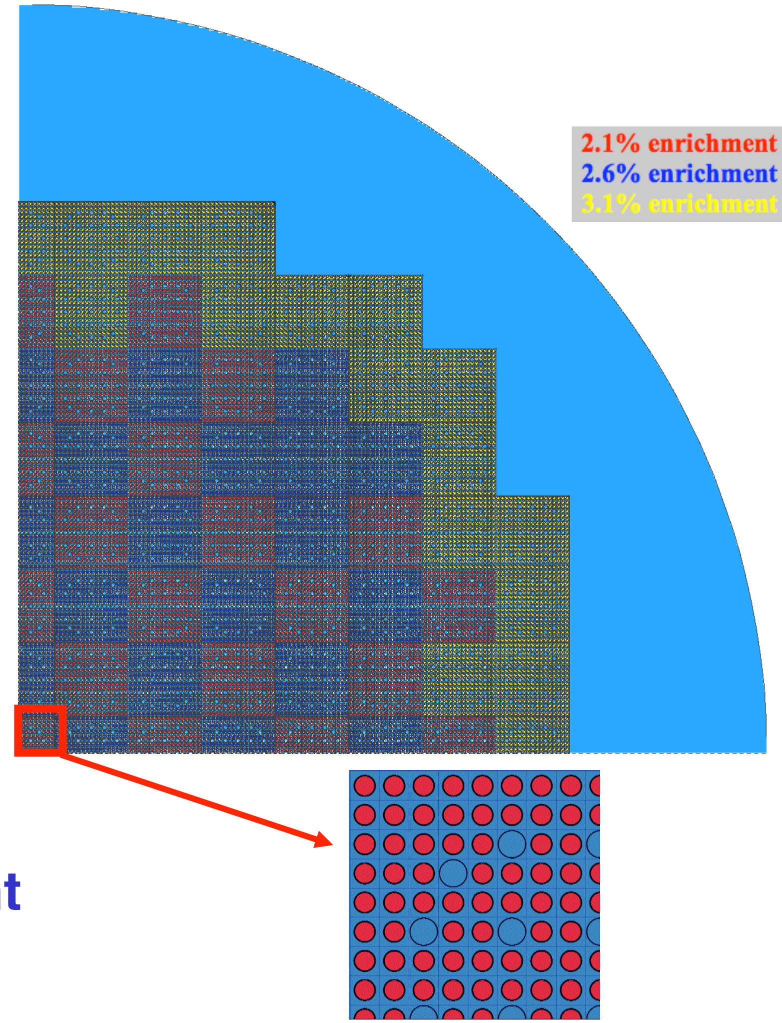
2D PWR (Nakagawa & Mori model)

- **48 1/4 fuel assemblies:**
  – 12,738 fuel pins with cladding
  – 1206 1/4 water tubes for control rods or detectors
- **Each assembly:**
  – Explicit fuel pins & rod channels
  – 17x17 lattice
  – Enrichments: 2.1%, 2.6%, 3.1%
- **Dominance ratio ~ .98**
- **Calculations used whole-core model, symmetric quarter-core shown at right**
- **ENDF/B-VII data, continuous-energy**



For numerous other examples, see companion talk at this meeting:
Carney, et al, "Fission Matrix Capability for MCNP, Part II – Applications"

- **Next 2 slides:**
  - **Spatial mesh for fission matrix:**
    - 8 x 8 x 1 mesh per assembly
    - 120 x 120 x 1 overall mesh
    - **14,400 spatial regions**
  - **Eigenvalues & eigenfunctions from Matlab:**
    - For this **specific fission matrix size** of 14,400 x 14,400
    - Fission matrix has 207 M elements = 1.6 GB
    - Use Matlab to get all 14,400 eigenvalues & eigenvectors
      - Expensive, time-consuming – requires nonsymmetic eigensolver

PWR – Eigenmodes for 120x120x1 Spatial Mesh

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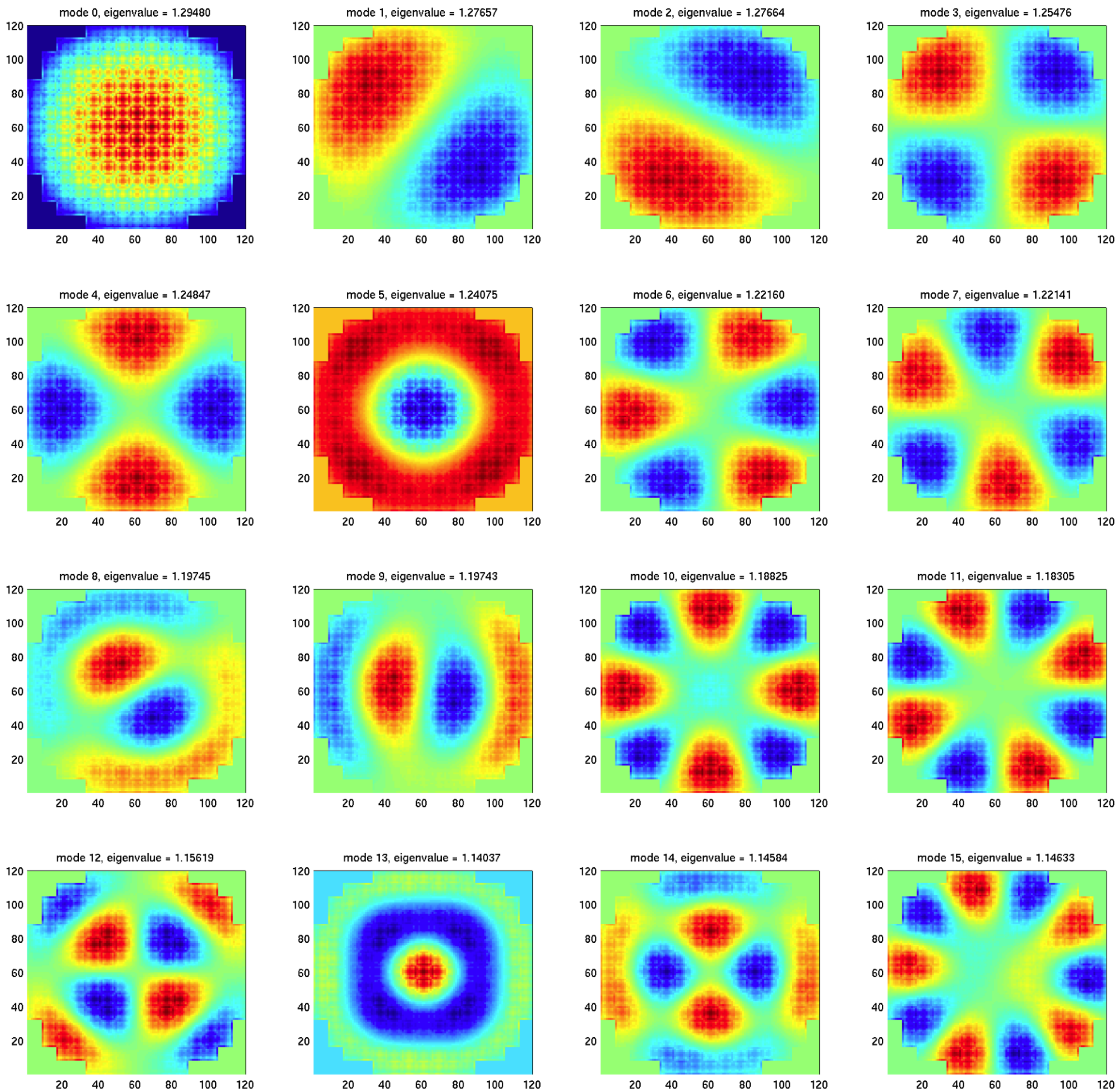
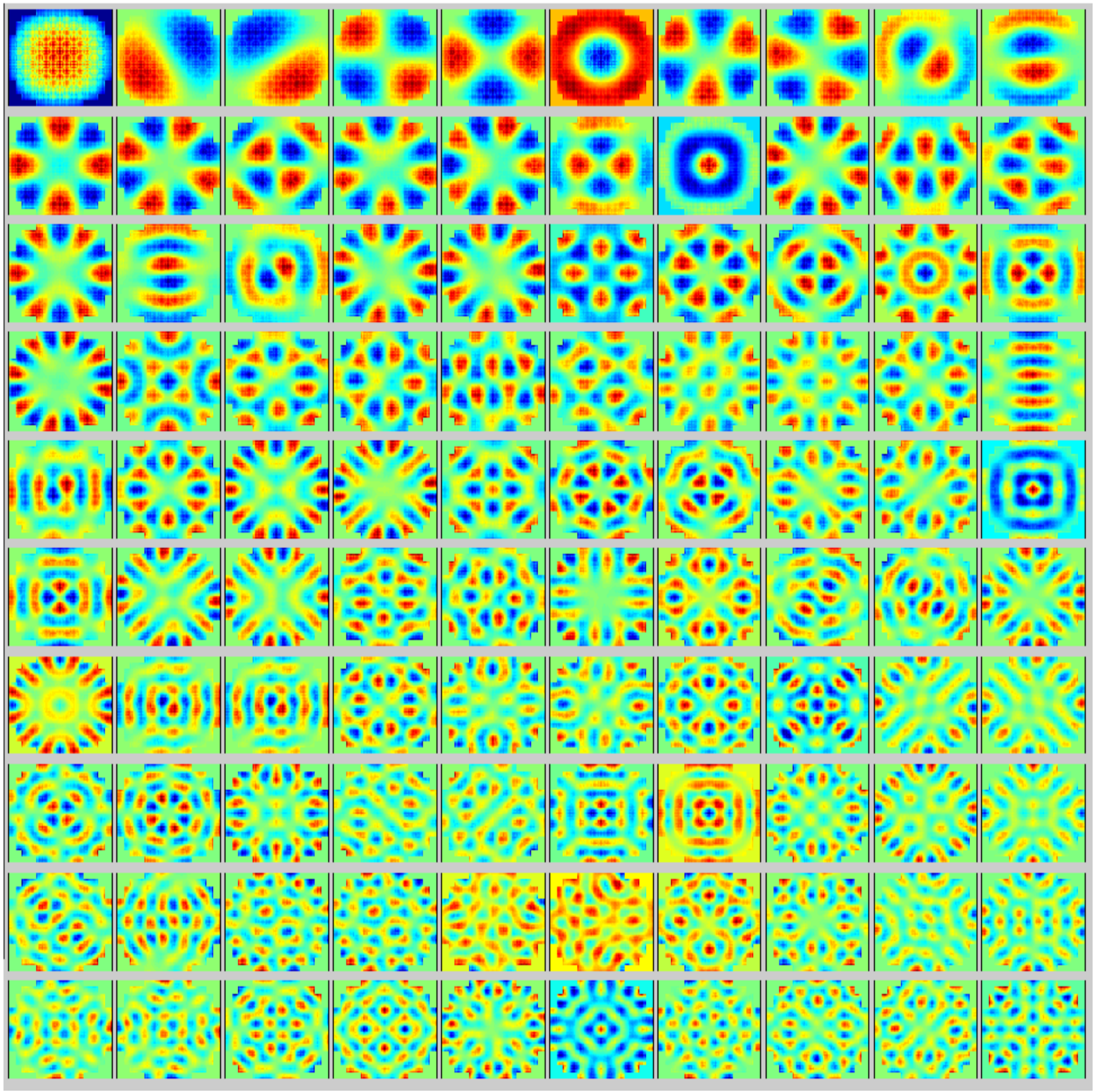


n	K_n
0	1.29480
1	1.27664
2	1.27657
3	1.25476
4	1.24847
5	1.24075
6	1.22160
7	1.22141
8	1.19745
9	1.19743
10	1.18825
11	1.18305
12	1.15619
13	1.14633
14	1.14617
15	1.14584

PWR – First 100 Eigenmodes, with More Neutrons



Fission Matrix Analysis of PWR Model

- **Following 2 slides:**
  - Vary the spatial discretization
  - Find eigenvalue spectrum for each discretization
  - Examine eigenvalue spectrum vs number of spatial regions
    - N regions $\Rightarrow$ N eigenvalues
    - For small N, fewer eigenvalues to represent problem, inaccurate
  - As N increases, spectrum extends & converges smoothly
    - No anomalies, no oscillations
    - Provides measure of adequate mesh refinement
      for fission matrix accuracy

Eigenvalue Spectra with Varying Meshes

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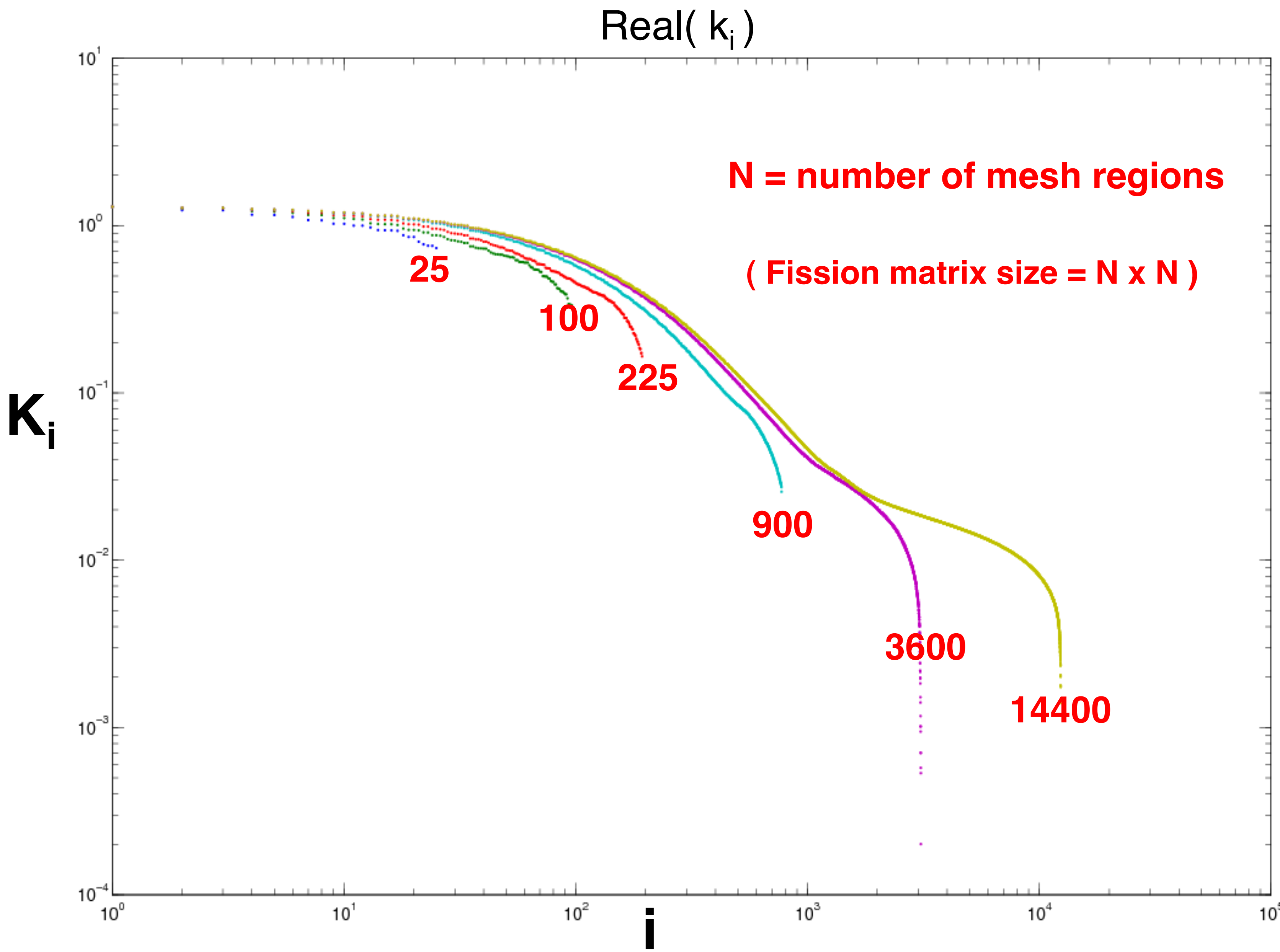
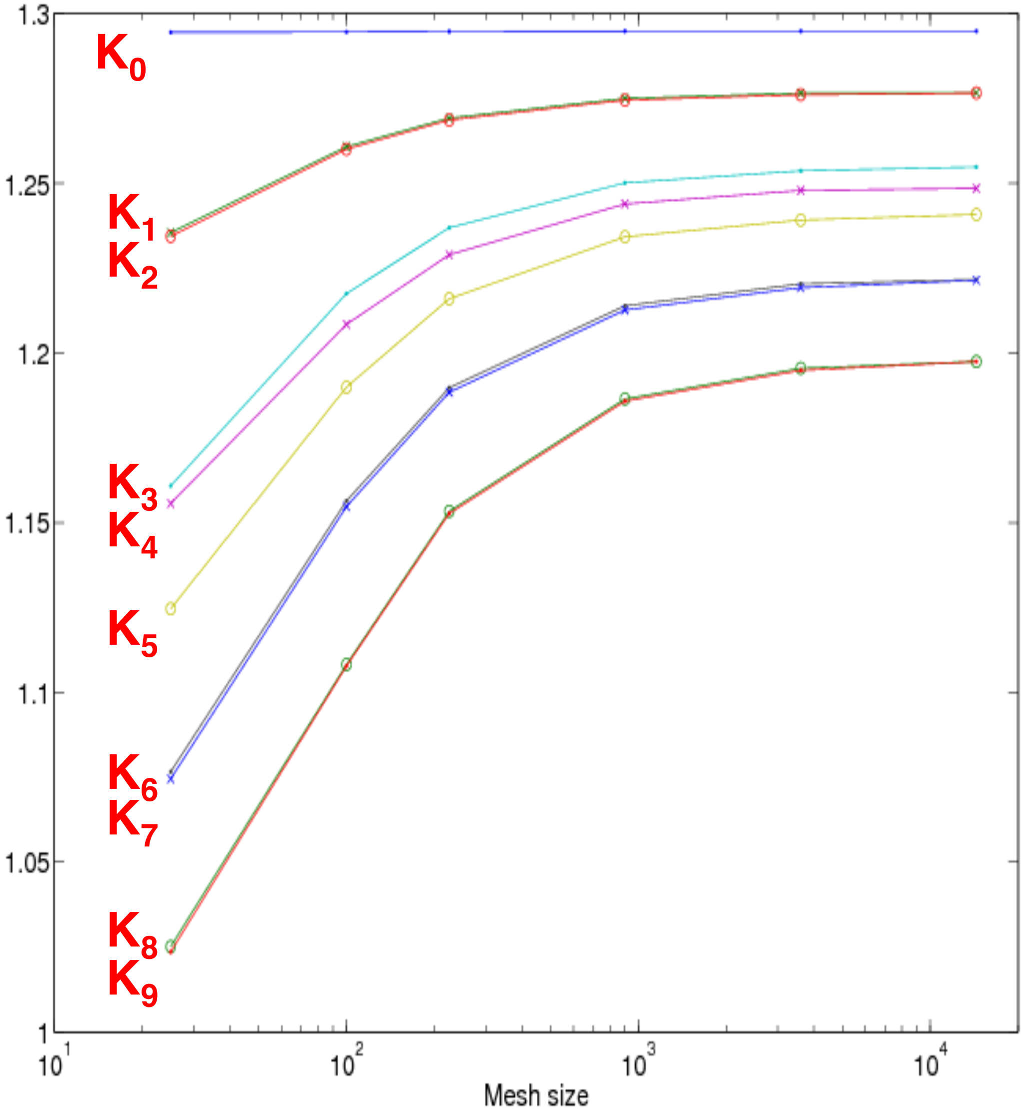


Spectrum Convergence from Mesh Refinement

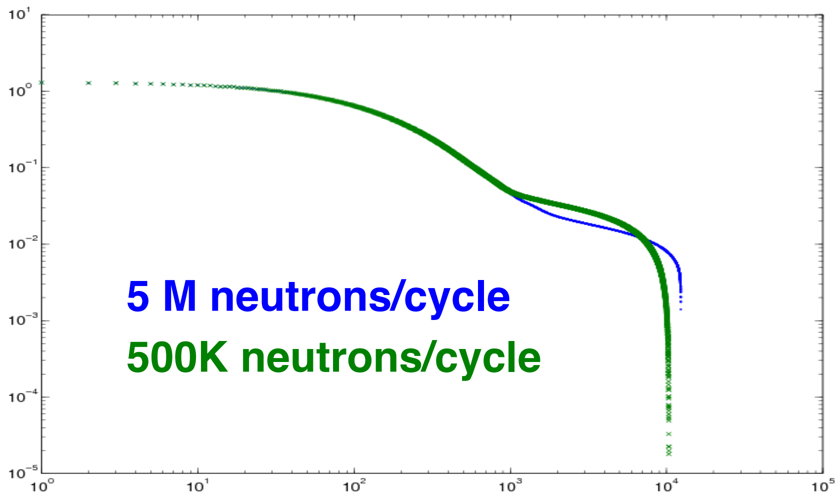


# Mesh Regions			K_0
5x5	=	25	1.29444
10x10	=	100	1.29453
15x15	=	225	1.29469
30x30	=	900	1.29477
60x60	=	3600	1.29479
120x120	=	14400	1.29480

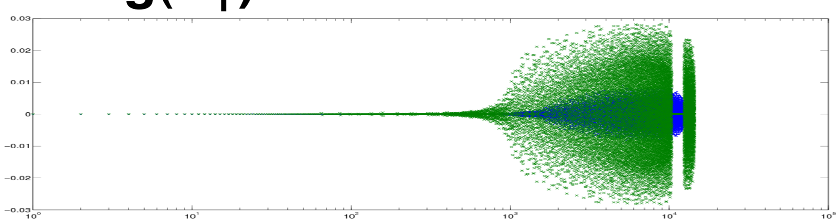
For fine-enough spatial mesh, eigenvalue spectrum converges

Are the Eigenvalues Real or Complex ?

Real(k_i):



Imag(k_i):

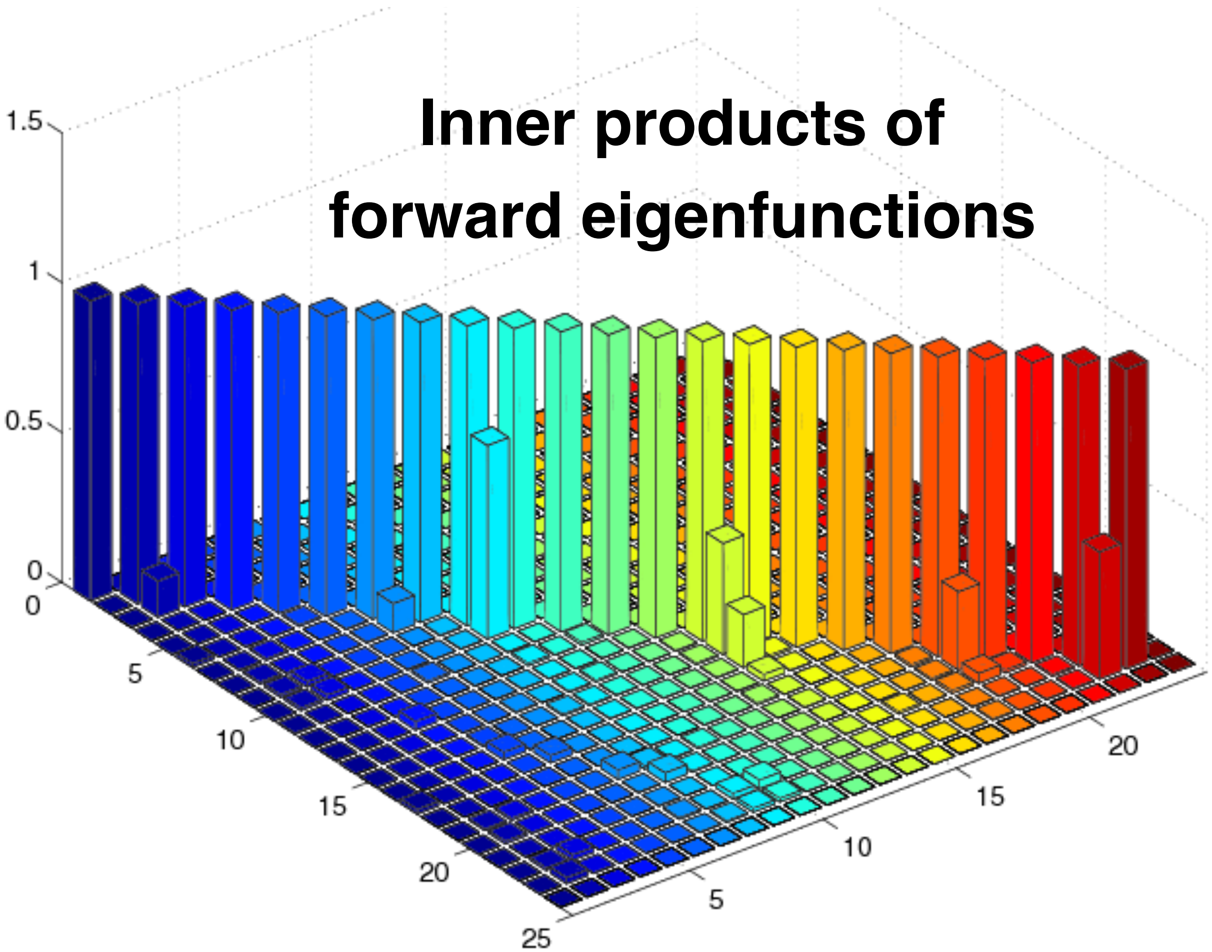


The appearance of complex eigenvalues appears to be strictly an artifact of Monte Carlo statistical noise

When more neutrons/cycle are used to decrease statistical noise, complex components diminish or vanish

The first few 100s or 1000s of discrete eigenvalues are real, and presumably <u>all</u> would be with sufficiently large neutrons/cycle

120 by 120 Spectrum, Varying Neutrons/cycle



$$\int d\vec{r}\,\psi_n(\vec{r})\psi_m(\vec{r})$$
$$= \delta_{nm}\ \ if\ \ fission\,kernel$$
$$is\ self\ adjoint/symmetric$$

Strictly, eigenfunctions of the transport equation are bi-orthogonal.

As shown above, forward eigenfunctions are very nearly orthogonal.

Conclusions
&
Future Work

Conclusions

- **Derived theory underlying fission matrix method**
  - **Rigorous Green's function approach, no approximations**
  - **Specific conditions on spatial resolution required for fission matrix accuracy**
  - **If spatial resolution fine enough, adjoint fission matrix identical to transpose of forward fission matrix**
- **Applied to realistic continuous-energy MC analysis of typical reactor models. Numerical evidence that:**
  - **Infinite set of discrete, real-valued eigenvalues & eigenfunctions exist for the integral fission neutron source & adjoint**
  - **As spatial resolution is refined, eigenvalue spectrum converges smoothly**
  - **While forward & adjoint are biorthogonal, forward modes are very nearly self-adjoint (for reactor-like problems)**

Future Work

- **Use fission matrix to accelerate source convergence**
  – Already demonstrated;   very effective;   needs work to automate

- **Use fission matrix for automatic, on-the-fly determination of source convergence**
  – Automate the determination of "inactive cycles"

- **Use fission matrix to assess problem coverage**
  – Need more neutrons/cycle to get adequate tallies?

- **Higher modes can be used to reduce/eliminate cycle-to-cycle correlation bias in statistics**
  – Replicas & ensemble statistics may be better, for exascale computers

- **Apply higher-mode analysis to reactor physics problems**
  – Xenon & void stability, slow transients, etc.

Questions ?

See Sean Carney's talk for more examples, applications, ideas